T. Oprea, P. Clemons, *Organizers*
R. Guha, *Organizer, Presiding*

8:50 Introductory Remarks.

8:55 . Pushing chemical biology data through the pipes: Architecting and extending the BARD API. **R. Guha**, J. Braisted, A. Jadhav, D. Nyguen, T. Peryea, N. Southall

9:20 . QSAR modeling on the web. **D. Pozefsky**, D. Deb, C. Xie, A. Sedykh, A. Tropsha

9:45 . Data curation and formal BioAssay Ontology (BAO)-based annotations of the DrugMatrix enable bioactivity-based target-relationship analysis and demonstrate incorporation of external datasets into the BioAssay Research Database (BARD). **T. Oprea**, S. Schurer, A. Mir, U. Vempati, J. Yang, O. Ursu, C. Bologa

10:10 Intermission.

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10:45 . BADAPPLE promiscuity plugin for BARD: Evidence-based promiscuity scores. **J. J. Yang**, O. Ursu, C. G. Bologa, A. Waller, L. A. Sklar, T. I. Oprea

11:10 Demo.

11:30 Panel Discussion.

T. Oprea, P. Clemons, *Organizers*
R. Guha, *Organizer, Presiding*

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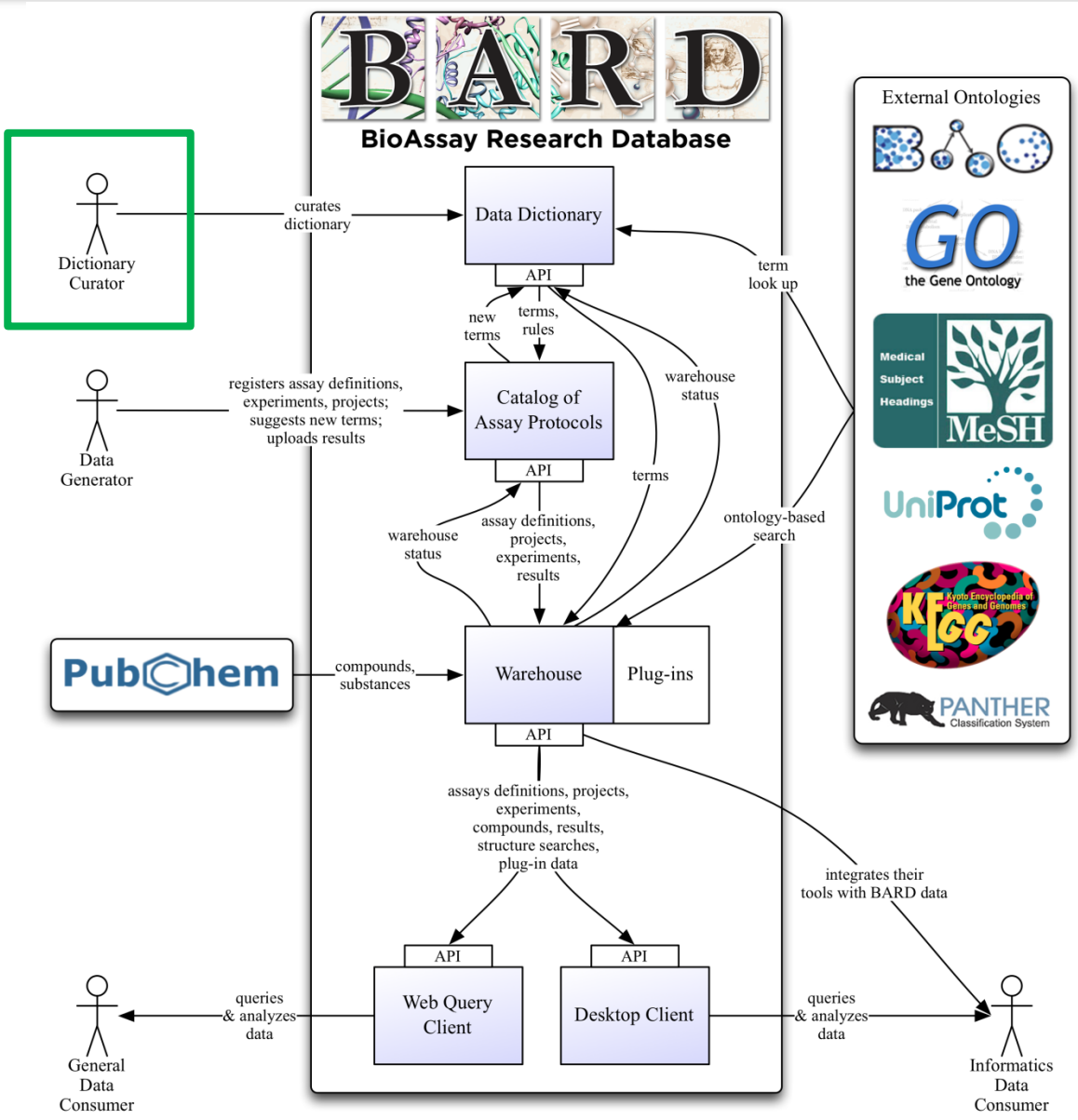
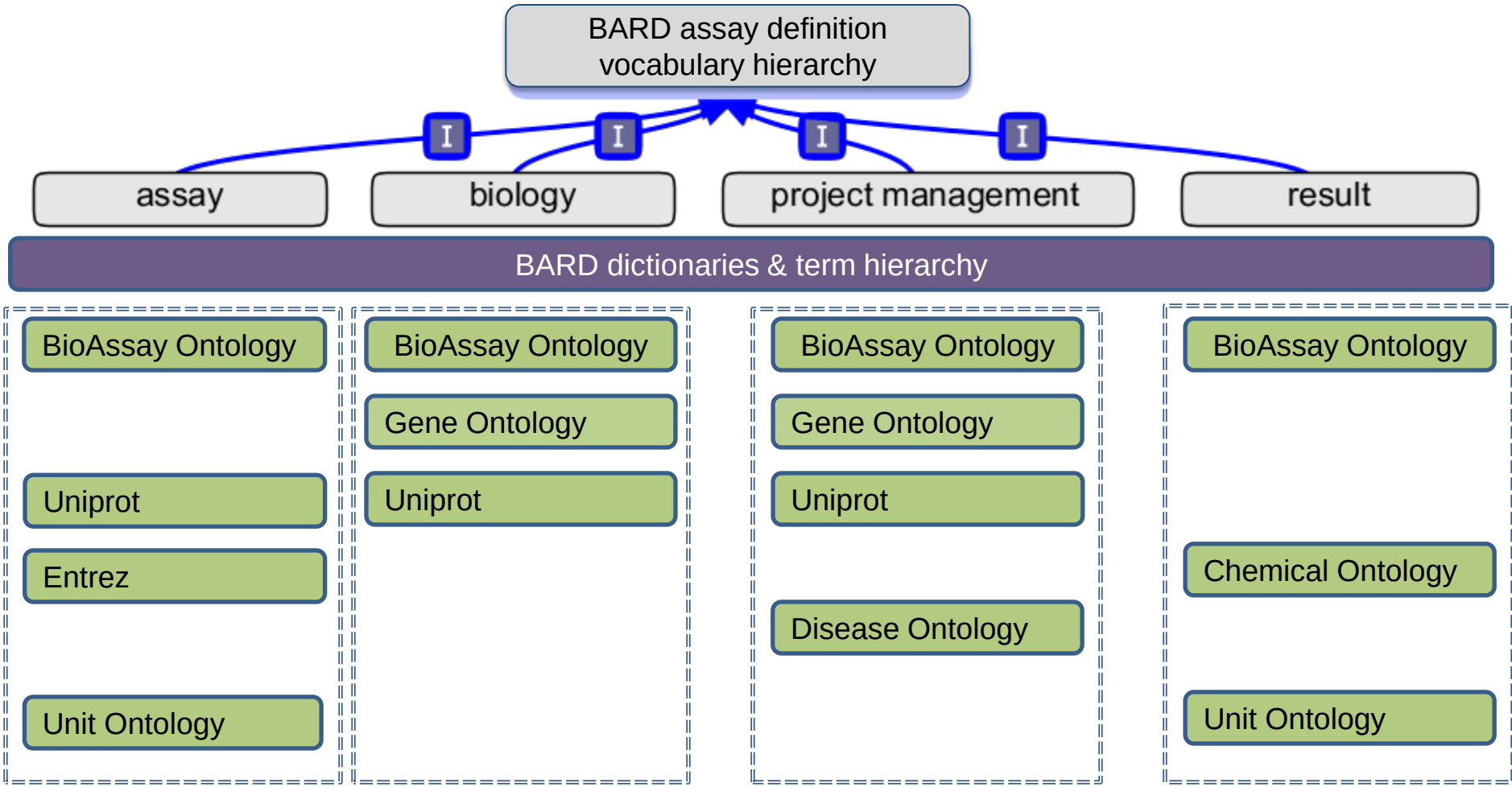
BARD is a fourth-generation small-molecule assay results DB

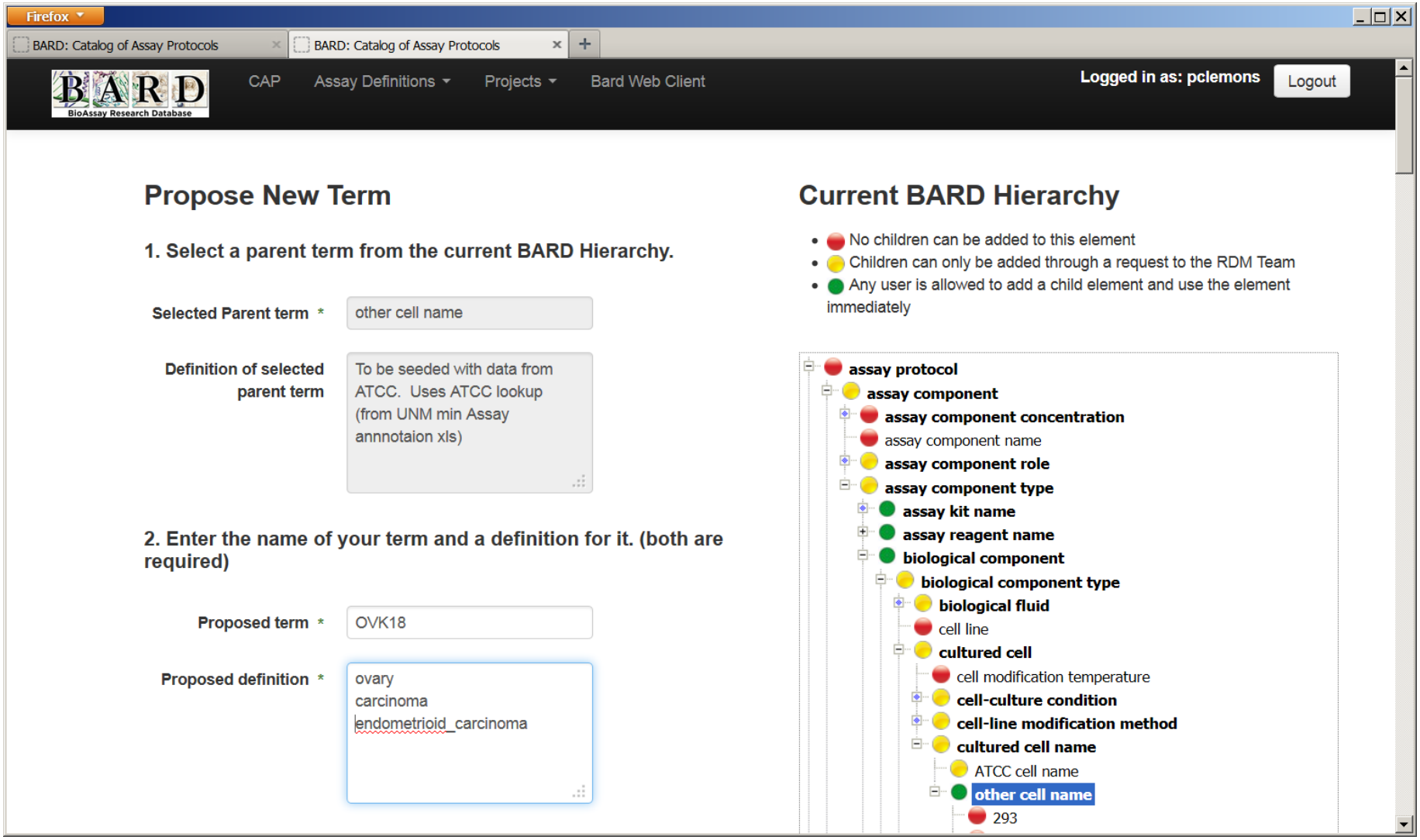
BARD addresses needs of multiple types of users



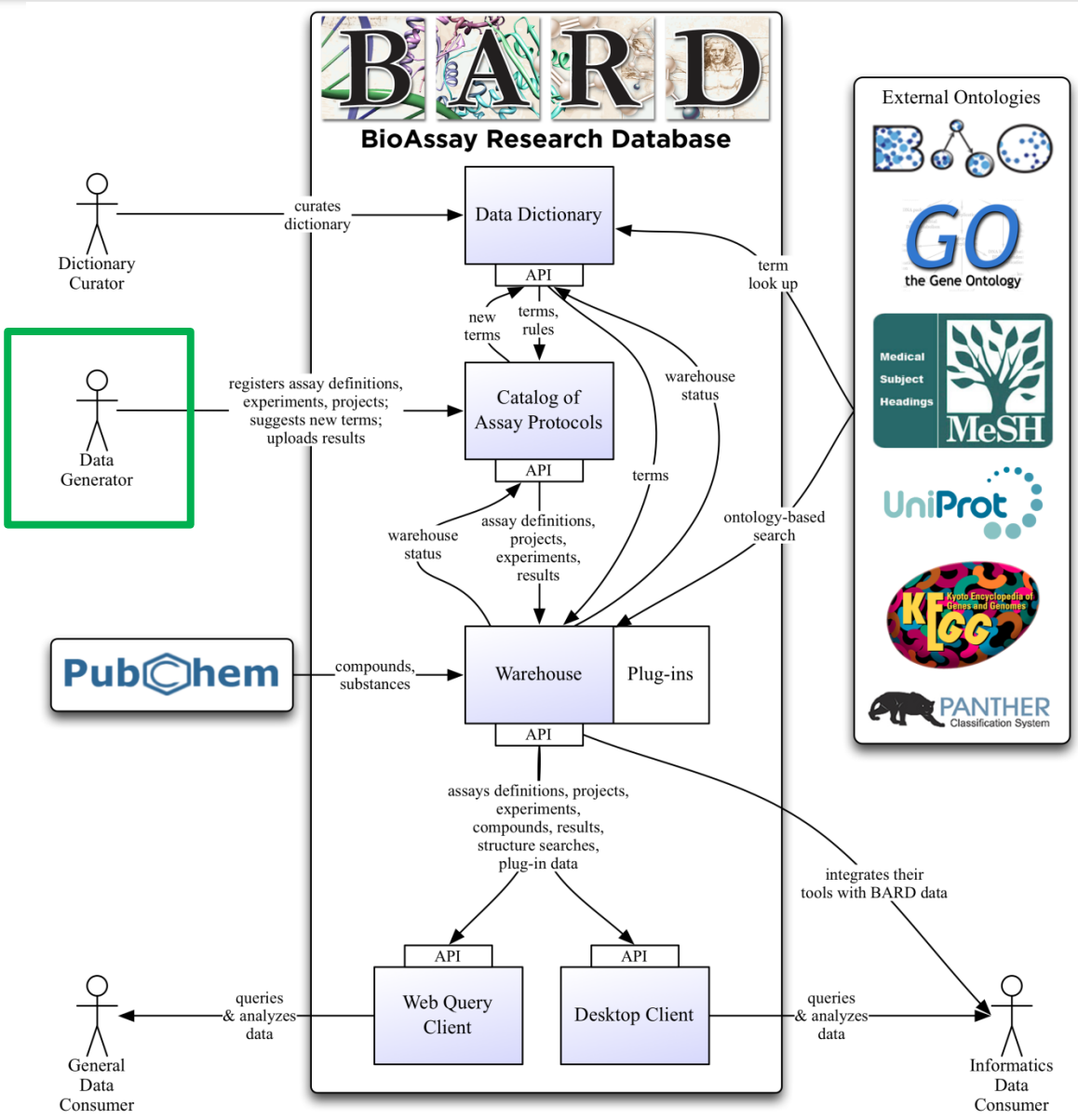
BARD combines custom and existing controlled vocabularies



BARD combines custom and existing controlled vocabularies



BARD addresses needs of multiple types of users



View Project (PID: 907)

1. Overview
2. Contexts
3. Experiments and steps
4. Documents
4.1. Descriptions
4.2. Protocols
4.3. Comments
4.4. Publications
4.5. External URLS
4.6. Others

1. Overview

PID: 907
Status: Approved
Name: Screen for RAS-Selective Lethal Compounds and VDAC Ligands
Description: Genetically matched immortalized cell lines expressing or not expressing HRAS-V12 were screened to identify compounds selectively lethal to cells expressing mutant HRAS. Two probe compounds, ML162 and ML210, were discovered.
Owner: Broad
Date Created: 05/19/2013
Last Updated: 08/09/2013
Modified By: dlahr

2. Contexts

project management	
laboratory name	Broad Institute
grant number	MH084117-01
assay provider name	(237) Brent Stockwell (Brent Stockwell)

biology	
GO biological process term	positive regulation of cell death
UniProt accession number	GTPase HRas
mutated protein	amino acid substitution
amino acid substitution	HRas V12G
disease	cancer
biology	biological process

probe	
PubChem CID	(3689413) SMR000206941 (CID 3689413)
probe report	ML162

probe	
PubChem CID	(49766530) TL_HRAS26 (CID 49766530)
probe report	ML210

Edit Contexts

3. Experiments and steps

1. Overview
2. Contexts
3. Experiments and steps
4. Documents
4.1. Descriptions
4.2. Protocols
4.3. Comments
4.4. Publications
4.5. External URLS
4.6. Others

Add Experiment | Link Experiments

Experiment Stage: confirmatory screen

Experiment ID: 3942 Remove from Project

Experiment Name:
HTS cherry pick confirmation at dose of HRas V12G synthetic lethal compounds

Assay Definition ID: 3947

PubChem AID: 1936

Click on an edge connecting experiments to see the details here.

View Experiment (3942)

Edit

1. Overview
2. Contexts
3. Measures
4. Documents
4.1. Descriptions
4.2. Protocols
4.3. Comments
4.4. Publications
4.5. External URLS
4.6. Others

1. Overview

EID: 3942
Assay Definition Luminescence Cell-Based Assay to Identify Compounds Cytotoxic to BJeLR RAS-Dependent Fibroblast
Status: Draft
Name: HTS cherry pick confirmation at dose of HRas V12G synthetic lethal compounds
Description: Confirmation at dose to identify compounds synthetically lethal in cells expressing HRas V12G. Viability is measured using Promega CellTiter Glo luminescent readout.
Owner: Broad
Run Date from: *Empty*
Run Date to: *Empty*
Date Created: 11/30/2012
Last Updated: 07/17/2013
Modified By: jbittker

External references

- PubChem aid=1936

Referenced by projects:

- Screen for RAS-Selective Lethal Compounds and VDAC Ligands

Download a template | Upload results | Reload Results from Pubchem

3. Measures

- EC50
  - (calculated from) percent activity
  - (supported by) Hill coefficient
  - (supported by) Hill s0
  - (supported by) Hill sinf
  - (supported by) percent activity (maximum)
  - (supported by) standard error
- PubChem outcome
  - (supported by) PubChem activity score

2. Contexts

number of replicates	
concentration-point number	8.0
number of replicates	2.0

activity threshold	
result detail	EC50
activity threshold	<150.0
unit	micromolar

project lead	
project lead name	Joshua A Bittker

activity threshold	
result detail	percent inhibition

View Assay Definition (ADID: 3947)

Clone Assay Definition

1. Overview
2. Biology
3. Assay Protocol
3.1. Assay Design
3.2. Assay Readout
3.3. Assay Components
3.4. Unclassified
4. Experiments
4.1. Experimental Variables
5. Measures
6. Documents
6.1. Descriptions
6.2. Protocols
6.3. Comments
6.4. Publications
6.5. External URLS
6.6. Others

1. Overview

ADID: 3947
Status: Approved
Name: Luminescence Cell-Based Assay to Identify Compounds Cytotoxic to BJeLR RAS-Dependent Fibroblast
Short Name:
Owner: Broad
Date Created: 11/30/2012
Definition Type: Regular
Version: 1.1
Last Updated: 08/23/2013
Modified By: gwalzer

2. Biology

biology	
biology	biological process
UniProt accession number	GTPase HRas
GO biological process term	(GO:0008219) cell death
mutated protein	amino acid substitution
amino acid substitution	HRas V12G

Edit Biology

3. Assay Protocol

assay format	
assay format	cell-based format
assay type	cytotoxicity assay

Edit Assay Protocol

3.1 Assay Design

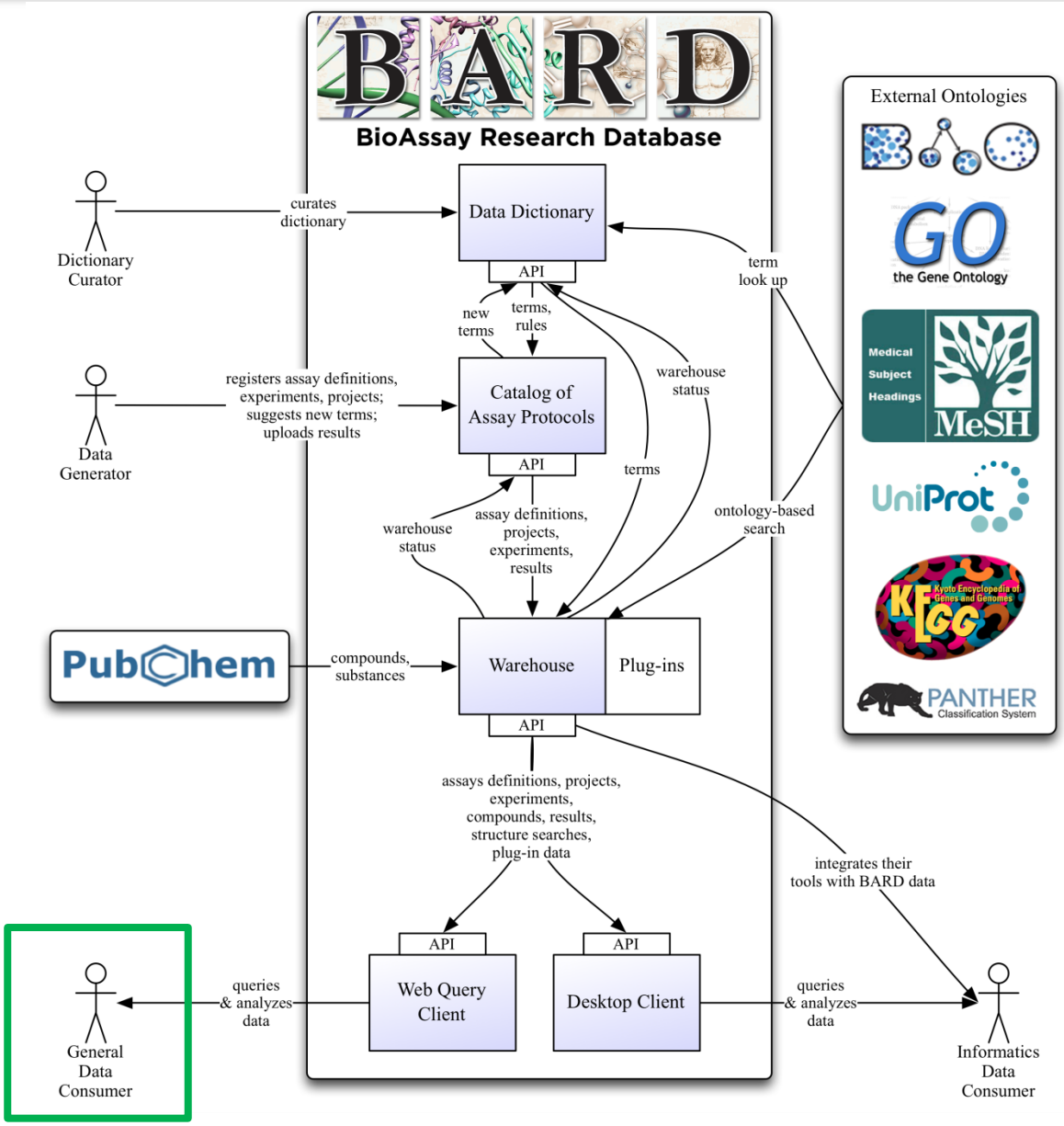
assay footprint	
assay footprint	384-well plate

Edit Assay Design

3.2 Assay Readout

detection method type	assay readout

BARD addresses needs of multiple types of users



BioAssay Research Database

RAS Search

Draw or paste a structure or list of IDs for search

Logged in as: **pclemons** Logout

Query Cart View/edit Visualize

Empty

Assay Definitions 203 | Compounds 15 | Projects 5

Clear All Filters | Apply Filters

Filters

Kegg disease category

- Cancer (1)
- Cardiac diseases (1)
- Developmental disorder (1)

Panther db protein class

- G-protein (1)
- enzyme modulator (1)
- small GTPase (1)

Num expt

- [5 TO 10] (3)
- [10 TO *] (3)

Previous | Next

Add All Items To Cart

Screen for RAS-Selective Lethal Compounds and VDAC Ligands (Project ID: 907)

Probe

Save to Cart for analysis

Search Match: Matched Field: Name

Number Of Experiments: 25

HTS to Identify Specific Small Molecule Inhibitors and Activators of Ras and Ras-Related GTPases (Project ID: 120)

Save to Cart for analysis

Search Match: Matched Field: Name

Number Of Experiments: 6

HTS to Identify Specific Small Molecule Inhibitors and Activators of Ras and Ras-Related GTPases (Project ID: 121)

Save to Cart for analysis

Search Match: Matched Field: Name

Number Of Experiments: 10

HTS to Identify Specific Small Molecule Inhibitors and Activators of Ras and Ras-Related GTPases (Project ID: 122)

Save to Cart for analysis

Search Match: Matched Field: Name

Number Of Experiments:

BioAssay Research Database

ras Search

Draw or paste a structure or list of IDs for search

Logged in as: **pclemons** Logout

Query Cart View/edit Visualize

Empty

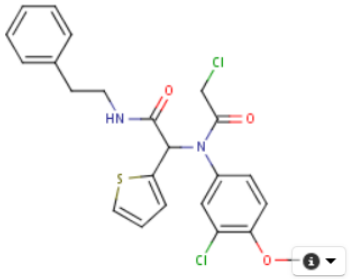
Probes
Annotations
Biology (4)
Description
Project Steps
Experiments (25)

Project: Screen for RAS-Selective Lethal Compounds and VDAC Ligands Probe (Project ID: 907)

Save to Cart for analysis

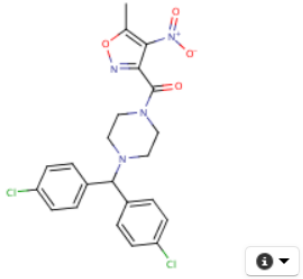
View in CAP

Probes



Probe ML#: ML162

- Download probe report from Molecular Library BookShelf
- Show Compound Details in BARD
- View CID 3689413 in PubChem
- Show Experimental Details



Probe ML#: ML210

- Download probe report from Molecular Library BookShelf
- Show Compound Details in BARD
- View CID 49766530 in PubChem
- Show Experimental Details

Annotations

probe	
PubChem CID	49766530
probe report	ML210

probe	
PubChem CID	3689413
probe report	ML162

project management	
laboratory name	Broad Institute
grant number	MH084117-01
assay provider name	(237) Brent Stockwell (Brent Stockwell)

biology	
GO biological process	positive regulation of cell death

Firefox

BioAssay Research Database

BioAssay Research Database

Similarity:3689413 threshold:90 Search

Draw or paste a structure or list of IDs for search

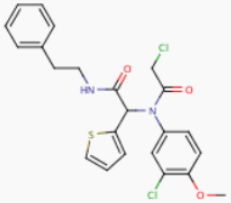
Logged in as: **pclemons** Logout

Query Cart View/edit Visualize

Empty

Assay Definitions (0) | Compounds 3 | Projects (0)

Add All Items To Cart



ML162 (PubChem CID: 3689413) Probe

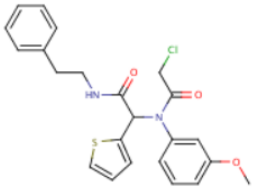
Save to Cart for analysis

Assays - Active vs Tested:

22 /119

Scaffold Promiscuity Analysis:

286	142	115	61	23
Show details	Show details	Show details	Show details	Show details



HMS2512I06 (PubChem CID: 3689415)

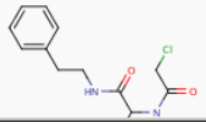
Save to Cart for analysis

Assays - Active vs Tested:

11 /110

Scaffold Promiscuity Analysis:

286	142	115	61	23
Show details	Show details	Show details	Show details	Show details



HMS2512I04 (PubChem CID: 3689416)

Save to Cart for analysis

Assays - Active vs Tested:

BioAssay Research Database

Search

Draw or paste a structure or list of IDs for search

Logged in as: **pclemons** Logout

Query Cart View/edit Visualize

3 compounds

Molecular Spreadsheet

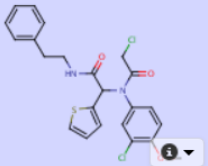
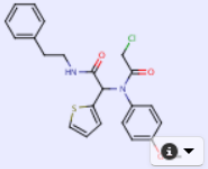
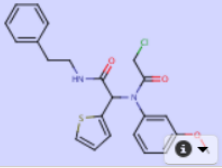
Please note: Only active compounds are shown in the Molecular Spreadsheet

☑ Hide Promiscuity Scores

T Transpose columns and rows

Show 10 entries

Search:

Molecular structure	CID	Active vs Tested across all Assay Definitions	ADID=3947 Denormalize		ADID=1125 Denormalize			ADID=1121 Denormalize			ADID=951 Denormalize
			percent activity	EC50	EC50	EC50	AC50	EC50	EC50	AC50	AC50
	3689413	22 / 119	140 139	N.T.	0.0340	0.0253 uM	0.232 uM	< 0.104 uM 0.0242 uM	0.0260	0.249 uM	10 uM
	3689416	16 / 115	110 118	2.97 uM	0.214	0.447 uM	N.T.	0.504 uM 0.363 uM	0.217	N.T.	10 uM
	3689415	11 / 110	82.4 61.7	N.T.	0.145	0.28 uM	N.T.	0.25 uM 0.179 uM	0.168	N.T.	10 uM

BioAssay Research Database

ras Search

Draw or paste a structure or list of IDs for search

Logged in as: **pclemons** Logout

Query Cart View/edit Visualize

Empty

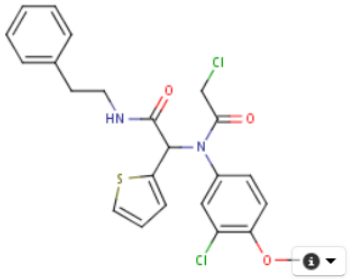
Probes
Annotations
Biology (4)
Description
Project Steps
Experiments (25)

Project: Screen for RAS-Selective Lethal Compounds and VDAC Ligands Probe (Project ID: 907)

Save to Cart for analysis

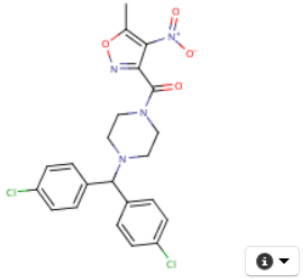
View in CAP

Probes



Probe ML#: ML162

- Download probe report from Molecular Library BookShelf
- Show Compound Details in BARD
- View CID 3689413 in PubChem
- Show Experimental Details



Probe ML#: ML210

- Download probe report from Molecular Library BookShelf
- Show Compound Details in BARD
- View CID 49766530 in PubChem
- Show Experimental Details

Annotations

probe	
PubChem CID	49766530
probe report	ML210

probe	
PubChem CID	3689413
probe report	ML162

project management	
laboratory name	Broad Institute
grant number	MH084117-01
assay provider name	(237) Brent Stockwell (Brent Stockwell)

biology	
GO biological process	positive regulation of cell death

BioAssay Research Database

Search

Draw or paste a structure or list of IDs for search

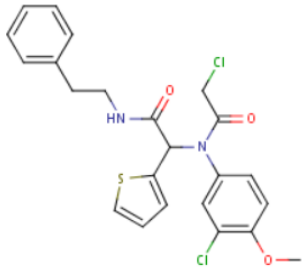
Logged in as: **pclemons** Logout

Query Cart View/edit Visualize

3 compounds

Linked Hierarchy Visualization

Compound Bio Activity Summary (cid: 3689413)



Group-by: PROJECT Group

Clear All Filters Apply Filters

Options

Plot axis

- [x] Normalize Y-Axis

Single-point measurement

- [x] Hide single-point data

Result type

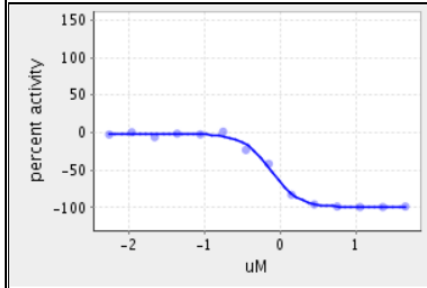
- [ ] AC50 (22)
- [ ] EC50 (10)
- [ ] percent activity (2)
- [ ] IC50 (1)

Only showing results where the compound is active

Please note: there is/are 6 experiment(s) with single-point data only

Please note: there is/are 7 experiment(s) with no data

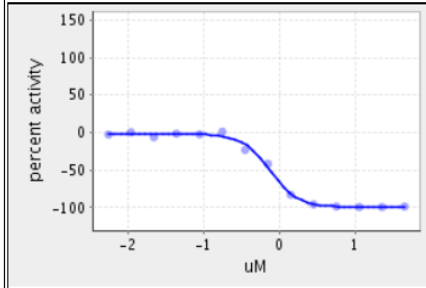
Project	Experiments
Screen for RAS-Selective Lethal Compounds and VDAC ... (907)	*Cytotoxicity counterscreen at dose of parental cell ... (1124)*



percent activity

-2.684E0 @ 5.600E-3 uM
2.890E-1 @ 1.110E-2 uM
-6.179E0 @ 2.220E-2 uM
-1.526E0 @ 4.400E-2 uM
-2.349E0 @ 8.900E-2 uM
1.015E0 @ 1.780E-1 uM
-2.315E1 @ 3.550E-1 uM
-4.169E1 @ 7.100E-1 uM
-8.310E1 @ 1.420E0 uM

Cytotoxicity counterscreen at dose of parental cell ... (1124)



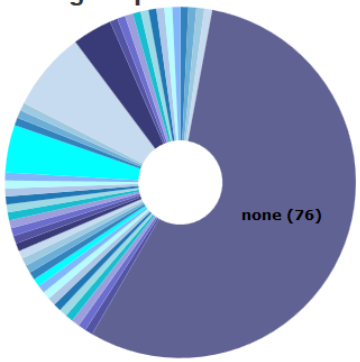
percent acti

-2.684E0 @ 5.60(
2.890E-1 @ 1.11(
-6.179E0 @ 2.22(
-1.526E0 @ 4.40(
-2.349E0 @ 8.90(
1.015E0 @ 1.78(
-2.315E1 @ 3.55(
-4.169E1 @ 7.10(
-8.310E1 @ 1.42

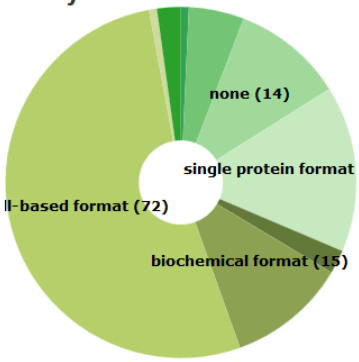
Firefox

Linked Hierarchies

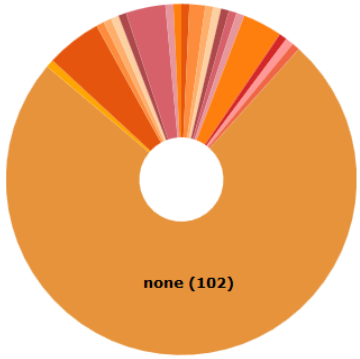
Biological process



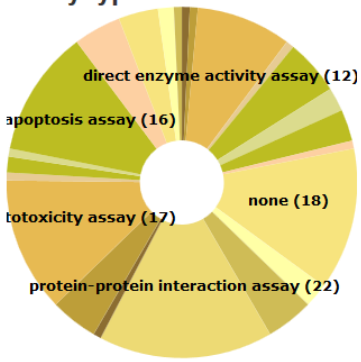
Assay format



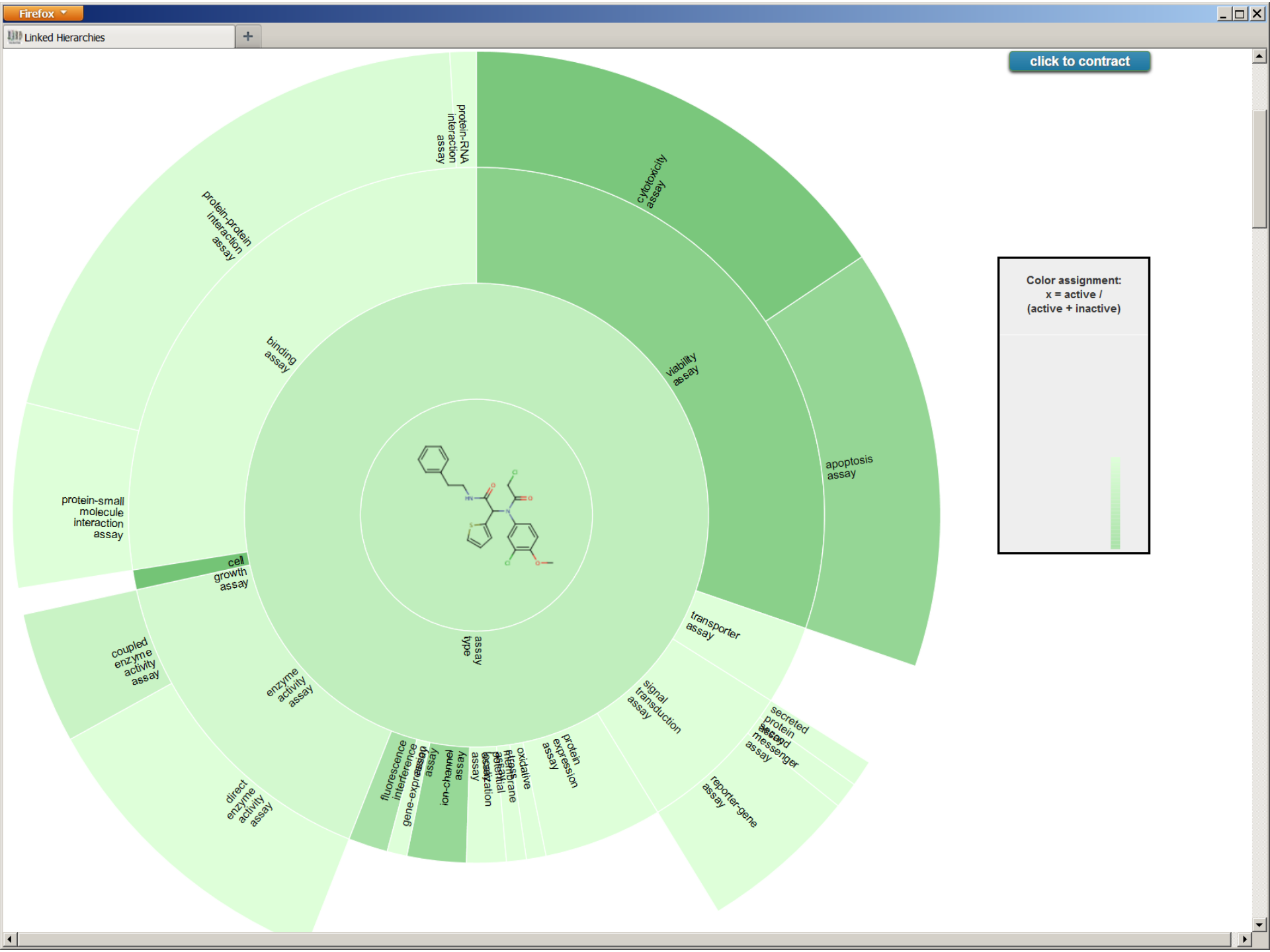
Protein class



Assay type

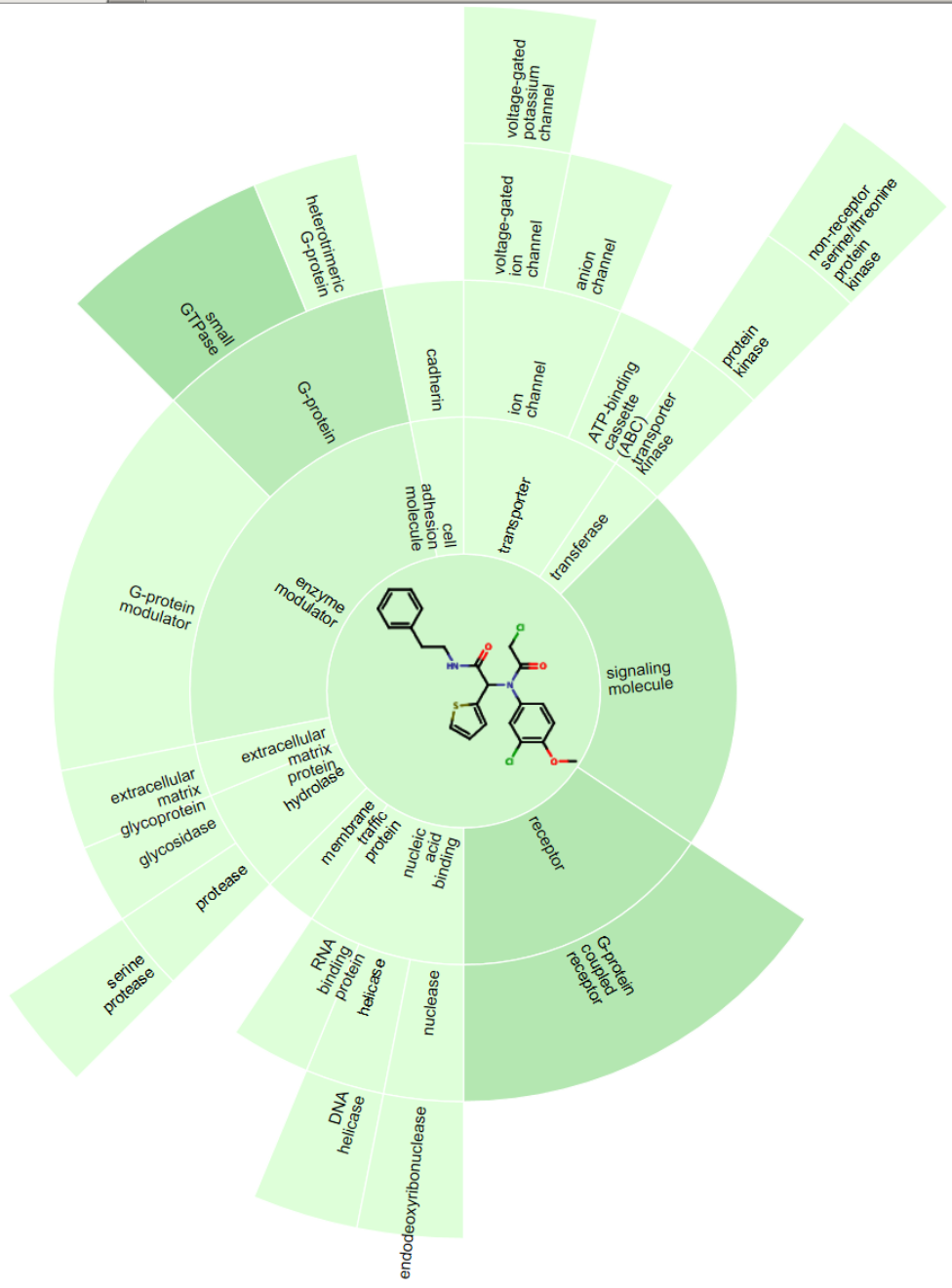


Biological process Drill down	Assay format Drill down	Protein class Drill down	Assay type Drill down	ADID
(6622) synuclein, alpha (non A4 component of amyloid precursor) [Homo sapiens]	cell-based format	none	reporter-gene assay	3901
(GO:0008219) cell death	cell-based format	none	cell growth assay	1675
(GO:0010544) negative regulation of platelet activation	cell-based format	G-protein coupled receptor	secreted protein assay	4013
ERK1 and ERK2 cascade	cell-based format	none	second messenger assay	3730
activation of cysteine-type endopeptidase activity involved in apoptotic process	cell-based format	signaling molecule	apoptosis assay	871
activation of cysteine-type endopeptidase activity involved in apoptotic process	cell-based format	none	apoptosis assay	576
activation of cysteine-type endopeptidase activity involved in apoptotic process	cell-based format	none	apoptosis assay	582
activation of cysteine-type endopeptidase activity involved in apoptotic process	cell-based format	none	apoptosis assay	1025
activation of cysteine-type endopeptidase activity involved in apoptotic process	cell-based format	none	apoptosis assay	1013
activation of cysteine-type endopeptidase activity involved in apoptotic process	cell-based format	none	apoptosis assay	1011
activation of cysteine-type				


Firefox
Linked Hierarchies
click to contract
Color assignment:
x = active /
(active + inactive)
assay type
binding assay
enzyme activity assay
viability assay
signal transduction assay
protein-RNA interaction assay
protein-protein interaction assay
protein-small molecule interaction assay
cell growth assay
coupled enzyme activity assay
direct enzyme activity assay
fluorescence interference assay
gene-expression assay
ion-channel assay
oxidative assay
protein expression assay
reporter-gene assay
secreted protein assay
second messenger assay
transporter assay
apoptosis assay
cytotoxicity assay

Firefox

Linked Hierarchies



BARD is large multi-Center collaborative project

T. Oprea, P. Clemons, *Organizers*
R. Guha, *Organizer, Presiding*

8:50 Introductory Remarks.

8:55 . Pushing chemical biology data through the pipes: Architecting and extending the BARD API. **R. Guha**, J. Braisted, A. Jadhav, D. Nyguen, T. Peryea, N. Southall

9:20 . QSAR modeling on the web. **D. Pozefsky**, D. Deb, C. Xie, A. Sedykh, A. Tropsha

9:45 . Data curation and formal BioAssay Ontology (BAO)-based annotations of the DrugMatrix enable bioactivity-based target-relationship analysis and demonstrate incorporation of external datasets into the BioAssay Research Database (BARD). **T. Oprea**, S. Schurer, A. Mir, U. Vempati, J. Yang, O. Ursu, C. Bologa

10:10 Intermission.

10:20 . Development of the BioAssay Research Database (BARD): A user-friendly perspective based on active participation from biologists and chemists. **E. S. Dawson**, S. R. Stauffer, C. W. Lindsley

10:45 . BADAPPLE promiscuity plugin for BARD: Evidence-based promiscuity scores. **J. J. Yang**, O. Ursu, C. G. Bologa, A. Waller, L. A. Sklar, T. I. Oprea

11:10 Demo.

11:30 Panel Discussion.

Panel Discussion – Talking Points 1

- Which type(s) of scientists represent BARD's primary use case and intended audience?
- Should BARD be optimized to suit particular groups of users (power-users, casual users)?

- How easy is it for users to get the information model (ADS) for their own research?
- What steps can users take to implement the BARD controlled vocabularies in their own research?
- To what extent do users just want raw data vs. processed data delivered via API?
- Can BARD data be used for mining and global analysis, or is it still easier to download data from PubChem?

Panel Discussion – Talking Points 2

- What differences should there be in the way BARD handles single-point HTS versus multi-point (e.g., concentration-response curve) data?
- Should data from primary assays be displayed alongside non-primary screens, or treated differently?

- How important are visualizations via the API? Should they be restricted to client applications?
- Are there other applications with which BARD should aim to integrate that are already optimized for certain types of data (e.g., GENE-E, Cytoscape)?
- Similar to the mechanism for adding back-end plug-ins, should BARD provide an extensible front end (to allow extensions of BARD's visual displays)?
- Could BARD be a general deployment platform for models, algorithms, vizualizations?

T. Oprea, P. Clemons, *Organizers*
R. Guha, *Organizer, Presiding*

8:50 Introductory Remarks.

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